

Characterization of Uncertainty in Thermophysical Properties Using Bayesian Inference

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In recent years, significant study has been conducted on the effect of uncertainty in thermophysical properties on process design and simulation. This is often done through the use of Monte Carlo techniques. Unfortunately, good experimental data over the entire range required are often not available and the uncertainty in the data which do exist is poorly specified if at all. For this reason a normal distribution is generally assumed for the uncertainty in the input properties with the width of the distribution based on expert opinion regarding the data.

Bayesian statistical analysis provides a rigorous mathematical basis for the inclusion of expert opinion to characterize uncertainty. This allows the analyst to infer a distribution for the uncertainty in a property based on experience and then include the data which do exist. This technique is often used in risk analysis and is extremely useful when there are few or no data for a property. As an example, non-normal distributions can easily be used to account for long tails in experimental properties resulting from impurities. Also, distributions for uncertainties in property prediction methods based on comparison to existing data can be developed and included in the assignment of uncertainties to values calculated using those methods. A framework for the use of Bayesian inference in physical property uncertainty characterization is presented and examples of its application provided.